

Ethanone, 1-(2,4-dihydroxyphenyl)-
89-84-9 | DTXSID4058998

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 127 °C

Global applicability domain: Inside

Local applicability domain index: 8.14e-01

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethanone, 1-(2,4-dihydroxyphenyl)-</div> <div>Measured: 146</div> <div>Predicted: 127</div>	<div>Image not found</div> <div>2',4'-Dihydroxypropiophenone</div> <div>Measured: 99.0</div> <div>Predicted: 110</div>	<div>Image not found</div> <div>2,4-Dihydroxybenzaldehyde</div> <div>Measured: 135</div> <div>Predicted: 127</div>
<div>Image not found</div> <div>Propiophenone, 2',5'-dihydroxy-</div> <div>Measured: 96.5</div> <div>Predicted: 108</div>	<div>Image not found</div> <div>2,3-Dihydroxybenzaldehyde</div> <div>Measured: 108</div> <div>Predicted: 113</div>	